Gamow states as continuous linear functionals over analytical test functions

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The space of analytical test functions ξ, rapidly decreasing on the real axis (i.e., Schwartz test functions of the type $\mathscr{S}$ on the real axis), is used to construct the rigged Hilbert space (RHS) $(\xi,\mathscr{H},\xi')$. Gamow states (GS) can be defined in RHS starting from Dirac's formula. It is shown that the expectation value of a self-adjoint operator acting on a GS is real. We have computed exactly the probability of finding a system in a GS and found that it is finite. The validity of recently proposed approximations to calculate the expectation value of self-adjoint operators in a GS is discussed. © *1996 American Institute of Physics.* [S0022-2488(96)00209-5]

I. INTRODUCTION

The proper treatment of the continuum and the inclusion of decaying states belonging to it in the definition of Green's functions of physical interest is a long-standing problem in various fields of physics. The mathematical consequences of the inclusion of the continuum in the scattering of particles by a central potential have been explored by Gamow long ago.[1] A modern review of the scattering theory can be found in Ref. 2 where the basic elements of the involved radial differential equations are presented in great detail. The use of these states, as it has been shown by Gamow,[1] is of central importance in building the physical interpretation of the α-decay mode of heavy atomic nuclei.[3] The so-called Gamow resonant states [for simplicity Gamow states (GS)] fulfill purely outgoing boundary conditions with an exponential behavior at infinity.[2] Several methods have been proposed since the publication of Gamow's work,[4] particularly in connection with the normalizability of Green's functions in the presence of GS and in the treatment of completeness relations.[5] The mathematical equivalence between some of these methods has been discussed recently and the correspondence between Bergreen's and Mittag-Lefler's representations has been explored at length.[6] Presently a rich literature is available regarding the application of these concepts to nuclear reactions and to nuclear structure problems.[7]

The amount of information about mathematical properties of representations which include GS is also very rich. The use of decaying states of complex energy in the framework of the Hamiltonian formalism, and the use of deformed contours to compute survival amplitudes, has been reported in Ref. 8 by Sudarshan and co-workers. The formulation of quantum mechanics in the rigged Hilbert space (RHS) has been also studied by Bohm.[9] In Ref. 10 it is shown that idealized resonances are described, within the RHS, by generalized eigenvectors of a self-adjoint Hamiltonian with complex eigenvalues and a Breit–Wigner energy distribution. Similar arguments have been advanced by Gadella.[11,12,13] Among the difficulties posed by the use of GS one can mention the appearance of the exponential catastrophe and the need to include nonphysical

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states of negative energy in the definition of GS by an integral on the real axis.[14] A nonrigorous cure for the exponential catastrophe would be the use of some regularization techniques, such as the one proposed by Zel'dovich.[15] However, and with reference to explicit numerical applications, the use of these techniques does not guarantee the stability of the results since the onset of the exponential dominance of the GS can manifest itself at physical scales.[5] Among the recent references on GS we shall mention the work of T. Berggren,[16] where the possibility of defining expectation values of operators in a resonant state is considered. In the present work we shall focus our attention on the mathematical aspects of representations which include Gamow states. At variance with the usually adopted approach, i.e., by using the class of functions known as Hardy class functions,[11–13] we shall use tempered ultradistributions.[17,–20] The space of analytical functionals ξ' (tempered ultradistributions) is the minimal space whose Fourier antitransform accomodates real exponential functions as distributions. In the first part of this work the definition of the space of analytical test functions ξ is given and the corresponding RHS is constructed. Then Dirac's formulation of quantum mechanics in RHS is shown, the structure of GS is given explicitly, and the norm of GS in RHS is calculated. The contribution of GS to $P(E)$, the probability distribution of a system at energy E, is obtained and the relation with the Breit–Wigner weighted energy distribution is studied. Next, some examples of GS as analytical functionals are given. Finally, a comparison with Berggren's results on expectation values with resonant states is presented.

II. THE RIGGED HILBERT SPACE $(\xi,\mathscr{H},\xi')$

Let us consider the space ξ of entire analytical test functions $\hat{\phi}(z)$ rapidly decreasing on the real axis, i.e., $\hat{\phi}(z)|_{y=0}=\phi(x)$ is a test function of the Schwartz space $\mathscr{S}$ (see Refs. 17–21).

The structure of a countable normed space of ξ is given by the family of norms

$$\|\hat{\phi}\|_n=\sup_{|z|=n}|\hat{\phi}(z)|,\quad n\in\mathscr{N}. \tag{1}$$

These norms are compatible since

$$\|\hat{\phi}\|_n<\|\hat{\phi}\|_{n+1}. \tag{2}$$

In ξ we define the scalar product

$$\langle\hat{\psi},\hat{\phi}\rangle=\int_{-\infty}^{+\infty}dE\ \overline{\hat{\psi}(E)}\,\hat{\phi}(E) \tag{3}$$

and the norm

$$\|\hat{\phi}\|^2=\langle\hat{\phi},\hat{\phi}\rangle. \tag{4}$$

The space ξ is completed by using the norm of Eq. (4); the resulting space is the Hilbert space $\mathscr{H}$ of square-integrable functions ($\xi\subset\mathscr{H}$).

If ξ' are linear continuous functionals (distributions) over ξ, we have (Refs. 17–21)

$$\xi\subset\mathscr{H}\subset\xi'. \tag{5}$$

Here ξ is a nuclear space (see Ref. 22) and $(\xi,\mathscr{H},\xi')$ is a RHS or a Guelfand's triplet (GT). In this RHS a linear and symmetric operator A acting on ξ, which admits a self-adjoint prolongation $\overline{A}$ acting on $\mathscr{H}$, has a complete set of eigen-functionals on ξ' with real generalized eigenvalues.[23,24] Let us introduce the GT $(\tilde{\xi},\mathscr{H},\tilde{\xi}')$ which is related to the GT given in Eq. (5) by the Fourier transform

$$\phi(t)=\mathscr{F}^{-1}\{\hat{\phi}(E)\}=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{iEt}\hat{\phi}(E)dE. \tag{6}$$

If $\hat{\psi}(E)\in\xi'$, we define $\psi(t)$ by

$$\langle\psi(t),\phi(t)\rangle=\frac{1}{2\pi}\langle\hat{\psi}(E),\hat{\phi}(E)\rangle. \tag{7}$$

Consequently, one has

$$\psi(t)=\mathscr{F}^{-1}\{\hat{\psi}(E)\} \tag{8}$$

with

$$\phi(t)\in\tilde{\xi},\quad \psi(t)\in\tilde{\xi}'. \tag{9}$$

The Schwartz space $\mathscr{S}'$ (of tempered distributions) is included in ξ' and in $\tilde{\xi}'$ ($\mathscr{S}'\subset\xi'$). The distributions of $\mathscr{S}'$ fulfill Dirac's formula[17]

$$S(x)=\int_{-\infty}^{+\infty}\delta(x-y)S(y)dy. \tag{10}$$

The extension to ξ' of Dirac's formula is given by[17]

$$\hat{\psi}_c(z)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}\frac{1}{E-z}\hat{\psi}(E)dE, \tag{11}$$

where

$$\hat{\psi}(E)=\hat{\psi}_c(E+i0)-\hat{\psi}_c(E-i0). \tag{12}$$

Related to the RHS $(\tilde{\xi},\mathscr{H},\tilde{\xi}')$ [and $(\xi,\mathscr{H},\xi')$], it exists the abstract GT $(\xi_a,\mathscr{H}_a,\xi'_a)$. This relation is established with the help of the operator $\hat{x}$, representing in $\mathscr{H}_a$ the position operator x of $\mathscr{H}$. The operator $\hat{x}$ has a complete set of eigenfunctions in ξ'_a. We use for them Dirac's notation $|x\rangle$. To each abstract ket $|\phi\rangle\in\xi_a$ it corresponds a function $\langle x|\phi\rangle=\phi(x)\in\tilde{\xi}$. In other words, to each function $\phi(x)\in\tilde{\xi}$, it corresponds an abstract ket $|\phi\rangle\in\xi_a$, such that $\langle x|\phi\rangle=\phi(x)$. This procedure establishes the above-mentioned relation between ξ and ξ_a. When the space ξ is completed we obtain the Hilbert space $\mathscr{H}$, while the correspondence just established leads to the complete abstract space $\mathscr{H}_a(\supset\xi_a)$. Finally, any linear continuous functional ψ in $\tilde{\xi}'$ is made to correspond to that abstract ket, $|\psi\rangle\in\xi'_a$, such that

$$\psi(\phi)=\langle\psi|\phi\rangle \tag{13}$$

for all $\phi\in\tilde{\xi}$.

These relations represent Dirac's formalism of quantum mechanics in a RHS. For more details see the works cited in Ref. 25.

The principal difference between the triplets defined above and those considered in Ref. 11 are due to the fact that our space ξ is formed by ''ultra analytic'' test functions; i.e., any $\phi\in\xi$ is entire-analytic and rapidly decreasing on the real axis. The dual space ξ' is formed by ''ultradistributions'' (see Refs. 17–20). The space $\tilde{\xi}'$ is the minimal space that contains real exponentials. It also allows the representation of any ultradistribution by a pair of analytic functions that can be determined by Eqs. (11) and (12).

Let us now introduce a self-adjoint operator $H \in \mathscr{H}$, such that

$$H|E\rangle = E|E\rangle, \quad E_0 < E < E_1. \tag{14}$$

We shall consider all the $\hat{\psi} \in \xi'$ with support (in the sense of Ref. 17) in the interval (E_0, E_1). This means that $\hat{\psi}$ can be determined from the discontinuity $\psi(E)$ of the pair of analytic functions on the real axis. Furthermore, $\psi(E) = 0$ if $E \notin (E_0, E_1)$.

Following Eq. (11) one can write

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \hat{\psi}(E) dE \tag{15}$$

and

$$(\hat{\psi}(E_G))^* = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} (\hat{\psi}(E))^* \, dE \tag{16}$$

with

$$E_G = E_D + i\Gamma, \quad \Gamma > 0.$$

In Dirac's notation, $\hat{\psi}(E) = \langle E|\psi\rangle$. Thus

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|\psi\rangle dE, \tag{17}$$

$$(\hat{\psi}(E_G))^* = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} \langle \psi|E\rangle dE. \tag{18}$$

We can also write Eq. (17) as

$$\hat{\psi}(E_G) = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|dE|\psi\rangle.$$

We now define

$$\langle E_G| = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E - E_G} \langle E|dE \tag{19}$$

and

$$|E_G^*\rangle = \frac{1}{2\pi i} \int_{E_0}^{E_1} \frac{1}{E_G^* - E} |E\rangle dE. \tag{20}$$

In consequence,

$$\hat{\psi}(E_G) = \langle E_G|\psi\rangle, \tag{21}$$

$$(\hat{\psi}(E_G))^* = \langle \psi|E_G^*\rangle. \tag{22}$$

The state $|E_G^*\rangle$ is by definition a Gamow state. Note that if $\hat{\psi}(E)$ is the discontinuity of $\hat{\psi}_c(z)$ on the real axis, then $E^n \hat{\psi}(E)$ is the discontinuity of $z^n \hat{\psi}(z)$ also on the real axis.

Then we have [cf. Eq. (20)]

$$E_G{*}^n|E_G{*}\rangle=\frac{1}{2\pi i}\int_{E_0}^{E_1}\frac{1}{E_G{*}-E}E^n|E\rangle dE,$$

i.e.,

$$H^n|E_G{*}\rangle=\frac{1}{2\pi i}\int_{E_0}^{E_1}\frac{1}{E_G{*}-E}H^n|E\rangle dE \tag{23}$$

$$=E_G{*}^n|E_G{*}\rangle, \tag{24}$$

and $|E_G{*}\rangle$ is an eigenstate of H.

The states $|E_G{*}\rangle$ are normalizable and the norm is given by

$$\langle E_G|E_G^*\rangle=\frac{1}{4\pi^2\Gamma}\left[\arctan\left(\frac{E_1-E_D}{\Gamma}\right)-\arctan\left(\frac{E_0-E_D}{\Gamma}\right)\right]. \tag{25}$$

With this normalization, and for the $E_1\to\infty$ and $E_0\to-\infty$, the normalized GS can be cast in the more familiar form of Ref. 14.

In consequence, the diagonal matrix element of H between GS is given by the expression

$$\langle E_G|H|E_G^*\rangle=E_D+\frac{\Gamma}{2}\frac{\ln\left[\frac{(E_1-E_D)^2+\Gamma^2}{(E_0-E_D)^2+\Gamma^2}\right]}{\left[\arctan\left(\frac{E_1-E_D}{\Gamma}\right)-\arctan\left(\frac{E_0-E_D}{\Gamma}\right)\right]}. \tag{26}$$

With this result it is readily seen that the imaginary part of the diagonal matrix element satisfies

$$\mathrm{Im}\langle E_G|H|E_G^*\rangle=0, \tag{27}$$

and that for the limits $E_0\to-\infty$ and $E_1\to+\infty$ one has

$$\langle E_G|H|E_G^*\rangle=E_D. \tag{28}$$

The time evolution of a GS is given by

$$\langle\psi|e^{-iHt}|E_G{*}\rangle=e^{-iE_G{*}t}(\hat{\psi}(E_G))^* \tag{29}$$

as a consequence of Eqs. (11) and (23).

The probability distribution associated to a GS is given by

$$P(E)=|\langle E|E_G^*\rangle|^2=\frac{\Gamma}{(E-E_D)^2+\Gamma^2}\cdot\frac{1}{\left[\arctan\left(\frac{E_1-E_D}{\Gamma}\right)-\arctan\left(\frac{E_0-E_D}{\Gamma}\right)\right]}. \tag{30}$$

In the limit $E_1\to+\infty$, $E_0\to-\infty$, the above equation yields

$$P(E)=\frac{\Gamma/\pi}{(E-E_D)^2+\Gamma^2}, \tag{31}$$

which is the Breit–Wigner form proposed by Ref. 16.

Let us introduce the self-adjoint operator A, which is acting on $\mathscr{H}_a$,

$$A=\int_{-\infty}^{+\infty}|\lambda\rangle\lambda\, d\sigma_a(\lambda)\langle\lambda|, \tag{32}$$

where $\sigma_a(\lambda)$ is given by

$$\sigma_a(\lambda)=\begin{cases}\sum_{n=-\infty}^{+\infty}\Theta(\lambda-\lambda_n), & \lambda<\lambda_0\\ \lambda, \quad \lambda_0<\lambda<\lambda_1, & \end{cases} \tag{33}$$

and where Θ is a Heaviside step function. The expectation value of A between GS

$$\langle E_G|A|E_G{}^*\rangle=\int_{-\infty}^{+\infty}\langle E_G|\lambda\rangle\lambda\, d\sigma_a(\lambda)\langle\lambda|E_G{}^*\rangle \tag{34}$$

is real since $\langle E_G|\lambda\rangle = (\langle\lambda|E_G^*\rangle)^*$. So far, the results which we have presented are based on the use of the theory of tempered ultradistributions. In order to illustrate them we shall discuss some simple examples.

For the first case we have adopted the plane waves

$$\langle E|x\rangle=\frac{e^{-iEx}}{\sqrt{2\pi}}.$$

From Eq. (11) one obtains

$$\langle E_G|x\rangle=\sqrt{2\Gamma}\ \mathrm{sgn}[\mathrm{Im}(E_G)]e^{-iE_Gx} \tag{35}$$

for the wavefunction of a GS.[26]

The second example is given by the function

$$\langle E|x\rangle=[\Theta(E-E_0)-\Theta(E-E_1)]\frac{e^{-iEx}}{\sqrt{2\pi}},$$

and for this case Eq. (11) yields

$$\langle E_G|x\rangle=\frac{C}{2\pi i}[\ln(E_G-E_1)-\ln(E_G-E_0)]e^{-iE_Gx}, \tag{36}$$

where C is a constant.[26]

As it can be seen from these examples, the GS can be obtained as tempered ultradistributions.

III. BERGGREN APPROXIMATION

In the following we shall discuss the validity of the approximation proposed by Berggren[16] to calculate the expectation value of an operator in a resonant state. Following Berggren's notation, let us introduce the state $|k,\hat{k},l\rangle$ and the continuum wavefunction $\langle\mathbf{x}|k,\hat{k},l\rangle=\phi_k^{(+)}(\mathbf{r})$.

Then, since the energy E is given by

$$E(\mathbf{k})=\frac{k^2}{2m}, \tag{37}$$

the GS can be defined by

$$|E_G{}^*\rangle = \frac{\sqrt{\Gamma}}{i\sqrt{\pi/2}} \int_0^{+\infty} \frac{|E(\mathbf{k}),\hat{k},l\rangle}{E_G{}^* - E}\, dE. \tag{38}$$

One can write

$$|k,\hat{k},l\rangle = \sqrt{\frac{k}{m}}\, |E(\mathbf{k}),\hat{k},l\rangle \tag{39}$$

and, consequently,

$$|E_G{}^*\rangle = \frac{\sqrt{\Gamma}}{i\sqrt{\pi/2}} \int_0^{+\infty} \sqrt{\frac{k}{m}} \frac{|k,\hat{k},l\rangle}{E_G{}^* - E(\mathbf{k})}\, dk, \tag{40}$$

$$\langle E_G|A|E_G{}^*\rangle = \frac{2\Gamma}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk' \, \frac{\sqrt{kk'}}{m} \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{(E(\mathbf{k}') - E_G)(E(\mathbf{k}) - E_G{}^*)} \tag{41}$$

[see Eq. (2) of Ref. 16]. We are now in a position to compare the result provided by the present method, about the expectation value of an operator in a resonant GS, and Berggren's conjecture, namely,

$$\langle A\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle, \tag{42}$$

where

$$\langle E_G{}^*|A|E_G{}^*\rangle = \frac{2\Gamma}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk' \, \frac{\sqrt{kk'}}{m} \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{(E(\mathbf{k}') - E_G{}^*)(E(\mathbf{k}) - E_G{}^*)}. \tag{43}$$

The relation between Eqs. (40) and (42) can be expressed as

$$\begin{aligned}\langle A\rangle = \langle E_G|A|E_G{}^*\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle - \frac{2i\Gamma^2}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk' \, \frac{\sqrt{kk'}}{m} [E(\mathbf{k}) - E(\mathbf{k}')] \\ \times \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{|E(\mathbf{k}') - E_G|^2 |E(\mathbf{k}) - E_G|^2} \\ + \frac{4\Gamma^3}{\pi} \sum_{l,l'} \int_0^{+\infty} dk \int_0^{+\infty} dk' \, \frac{\sqrt{kk'}}{m} \frac{\langle k',\hat{k}',l'|A|k,\hat{k},l\rangle}{|E(\mathbf{k}') - E_G|^2 |E(\mathbf{k}) - E_G|^2}.\end{aligned} \tag{44}$$

It means that the result obtained by Berggren[16] is valid at leading order in Γ. At this order one obtains, from the above equation,

$$\langle A\rangle = \langle E_G|A|E_G{}^*\rangle = \mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle. \tag{45}$$

The contributions of higher-order terms, for any value of Γ, is given by Eq. (43). From this equation it is seen that the expectation value of the operator A in a GS differs from the estimate $\mathrm{Re}\langle E_G{}^*|A|E_G{}^*\rangle$ and that it shows a power-law dependence upon Γ.

IV. CONCLUSIONS

In this work we have presented a mathematical representation of GS based on the theory of tempered ultradistributions. The use of them has been shown to be useful, particularly in discussing the normalization of GS. The connection with Berggren's approximation, concerning the expectation value of an operator on a resonant state, has been established. We have shown that Berggren's expansion is valid at leading order in the imaginary part of the energy E_G. A general expression for this expectation value has been introduced which is not restricted by any prior assumption about the order of magnitude of the imaginary part of E_G as compared with the value of the real part of it. These results show that the space of ultradistributions together with the RHS discussed seems to be an appropriate framework for the description of GS and its main properties.

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